



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:38 AM GMT

PDB ID : 2XQY
Title : CRYSTAL STRUCTURE OF PSEUDORABIES CORE FRAGMENT OF GLYCOPROTEIN H IN COMPLEX WITH FAB D6.3
Authors : Backovic, M.; Dubois, R.; Cockburn, J.; Sharff, A.; Vaney, M.; Granzow, H.; Klupp, B.; Bricogne, G.; Mettenleiter, T.; Rey, F.
Deposited on : 2010-09-08
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

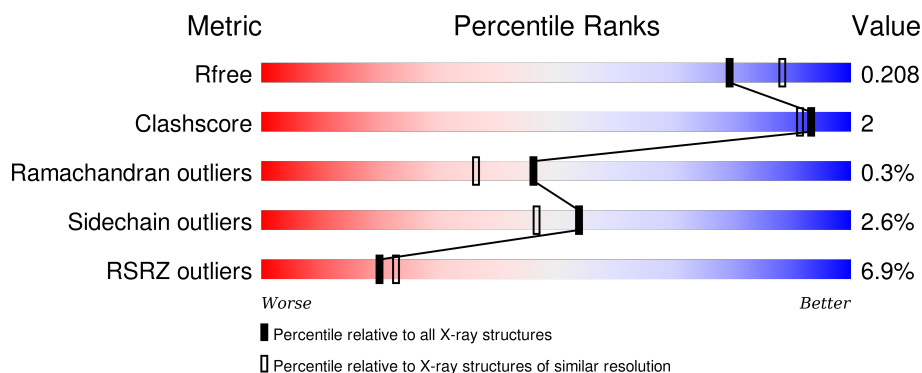
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	572	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>7%</div> <div>•</div> <div>19%</div> </div> </div>
1	E	572	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>6%</div> <div>•</div> <div>19%</div> </div> </div>
2	G	261	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>17%</div> </div> </div>
2	J	261	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>17%</div> </div> </div>
3	K	220	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>•</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	L	220	<div><div></div><div>2%</div><div>95%</div><div>5% •</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14739 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ENVELOPE GLYCOPROTEIN H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3475	2195	624	637	19			
1	E	464	Total	C	N	O	S	0	0	0
			3475	2195	624	637	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ARG	-	EXPRESSION TAG	UNP P27416
A	106	SER	-	EXPRESSION TAG	UNP P27416
A	640	PHE	-	EXPRESSION TAG	UNP P27416
A	641	GLU	-	EXPRESSION TAG	UNP P27416
A	642	ASP	-	EXPRESSION TAG	UNP P27416
A	643	ASP	-	EXPRESSION TAG	UNP P27416
A	644	ASP	-	EXPRESSION TAG	UNP P27416
A	645	ASP	-	EXPRESSION TAG	UNP P27416
A	646	LYS	-	EXPRESSION TAG	UNP P27416
A	647	ALA	-	EXPRESSION TAG	UNP P27416
A	648	GLY	-	EXPRESSION TAG	UNP P27416
A	649	TRP	-	EXPRESSION TAG	UNP P27416
A	650	SER	-	EXPRESSION TAG	UNP P27416
A	651	HIS	-	EXPRESSION TAG	UNP P27416
A	652	PRO	-	EXPRESSION TAG	UNP P27416
A	653	GLN	-	EXPRESSION TAG	UNP P27416
A	654	PHE	-	EXPRESSION TAG	UNP P27416
A	655	GLU	-	EXPRESSION TAG	UNP P27416
A	656	LYS	-	EXPRESSION TAG	UNP P27416
A	657	GLY	-	EXPRESSION TAG	UNP P27416
A	658	GLY	-	EXPRESSION TAG	UNP P27416
A	659	GLY	-	EXPRESSION TAG	UNP P27416
A	660	SER	-	EXPRESSION TAG	UNP P27416
A	661	GLY	-	EXPRESSION TAG	UNP P27416
A	662	GLY	-	EXPRESSION TAG	UNP P27416

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Chain	Residue	Modelled	Actual	Comment	Reference
A	663	GLY	-	EXPRESSION TAG	UNP P27416
A	664	SER	-	EXPRESSION TAG	UNP P27416
A	665	GLY	-	EXPRESSION TAG	UNP P27416
A	666	GLY	-	EXPRESSION TAG	UNP P27416
A	667	GLY	-	EXPRESSION TAG	UNP P27416
A	668	SER	-	EXPRESSION TAG	UNP P27416
A	669	TRP	-	EXPRESSION TAG	UNP P27416
A	670	SER	-	EXPRESSION TAG	UNP P27416
A	671	HIS	-	EXPRESSION TAG	UNP P27416
A	672	PRO	-	EXPRESSION TAG	UNP P27416
A	673	GLN	-	EXPRESSION TAG	UNP P27416
A	674	PHE	-	EXPRESSION TAG	UNP P27416
A	675	GLU	-	EXPRESSION TAG	UNP P27416
A	676	LYS	-	EXPRESSION TAG	UNP P27416
E	105	ARG	-	EXPRESSION TAG	UNP P27416
E	106	SER	-	EXPRESSION TAG	UNP P27416
E	105	ARG	-	EXPRESSION TAG	UNP P27416
E	106	SER	-	EXPRESSION TAG	UNP P27416
E	640	PHE	-	EXPRESSION TAG	UNP P27416
E	641	GLU	-	EXPRESSION TAG	UNP P27416
E	642	ASP	-	EXPRESSION TAG	UNP P27416
E	643	ASP	-	EXPRESSION TAG	UNP P27416
E	644	ASP	-	EXPRESSION TAG	UNP P27416
E	645	ASP	-	EXPRESSION TAG	UNP P27416
E	646	LYS	-	EXPRESSION TAG	UNP P27416
E	647	ALA	-	EXPRESSION TAG	UNP P27416
E	648	GLY	-	EXPRESSION TAG	UNP P27416
E	649	TRP	-	EXPRESSION TAG	UNP P27416
E	650	SER	-	EXPRESSION TAG	UNP P27416
E	651	HIS	-	EXPRESSION TAG	UNP P27416
E	652	PRO	-	EXPRESSION TAG	UNP P27416
E	653	GLN	-	EXPRESSION TAG	UNP P27416
E	654	PHE	-	EXPRESSION TAG	UNP P27416
E	655	GLU	-	EXPRESSION TAG	UNP P27416
E	656	LYS	-	EXPRESSION TAG	UNP P27416
E	657	GLY	-	EXPRESSION TAG	UNP P27416
E	658	GLY	-	EXPRESSION TAG	UNP P27416
E	659	GLY	-	EXPRESSION TAG	UNP P27416
E	660	SER	-	EXPRESSION TAG	UNP P27416
E	661	GLY	-	EXPRESSION TAG	UNP P27416
E	662	GLY	-	EXPRESSION TAG	UNP P27416
E	663	GLY	-	EXPRESSION TAG	UNP P27416

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Chain	Residue	Modelled	Actual	Comment	Reference
E	664	SER	-	EXPRESSION TAG	UNP P27416
E	665	GLY	-	EXPRESSION TAG	UNP P27416
E	666	GLY	-	EXPRESSION TAG	UNP P27416
E	667	GLY	-	EXPRESSION TAG	UNP P27416
E	668	SER	-	EXPRESSION TAG	UNP P27416
E	669	TRP	-	EXPRESSION TAG	UNP P27416
E	670	SER	-	EXPRESSION TAG	UNP P27416
E	671	HIS	-	EXPRESSION TAG	UNP P27416
E	672	PRO	-	EXPRESSION TAG	UNP P27416
E	673	GLN	-	EXPRESSION TAG	UNP P27416
E	674	PHE	-	EXPRESSION TAG	UNP P27416
E	675	GLU	-	EXPRESSION TAG	UNP P27416
E	676	LYS	-	EXPRESSION TAG	UNP P27416

- Molecule 2 is a protein called A13-D6.3 MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	216	Total	C	N	O	S	0	0	0
			1648	1044	270	327	7			
2	J	216	Total	C	N	O	S	0	0	0
			1648	1044	270	327	7			

- Molecule 3 is a protein called A13-D6.3 MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	218	Total	C	N	O	S	0	1	0
			1698	1059	288	344	7			
3	L	218	Total	C	N	O	S	0	0	0
			1689	1054	285	343	7			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

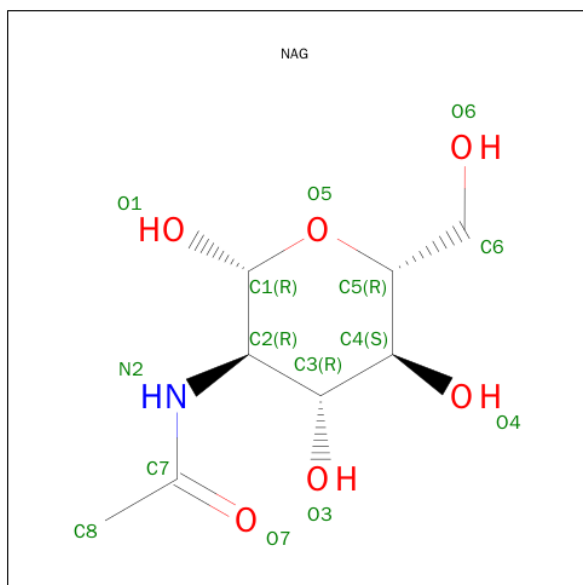
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

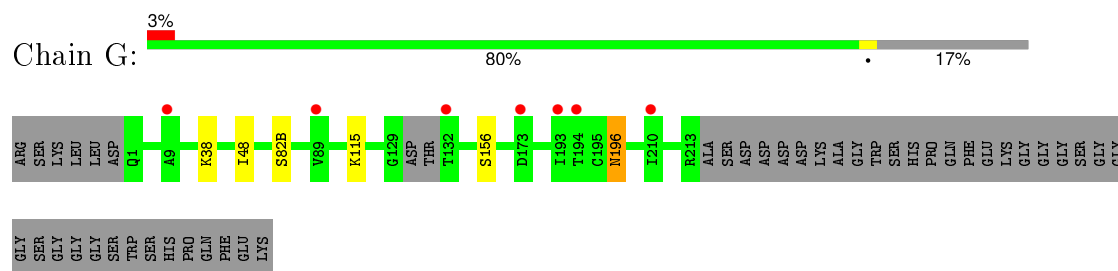


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

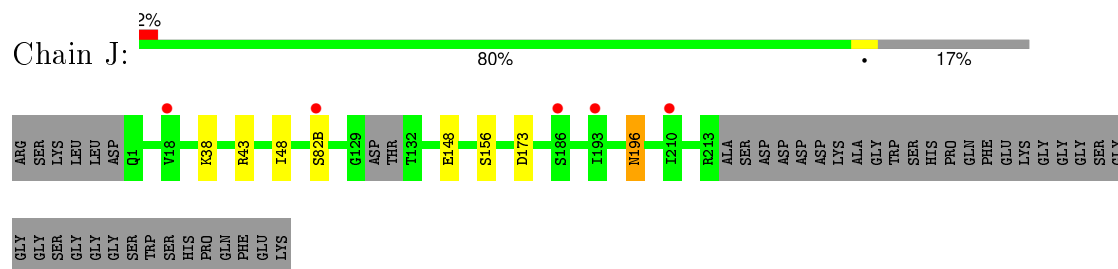
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total	O	0	0
			135	135		
6	E	159	Total	O	0	0
			159	159		
6	G	141	Total	O	0	0
			141	141		
6	J	184	Total	O	0	0
			184	184		
6	K	171	Total	O	0	0
			171	171		
6	L	162	Total	O	0	0
			162	162		

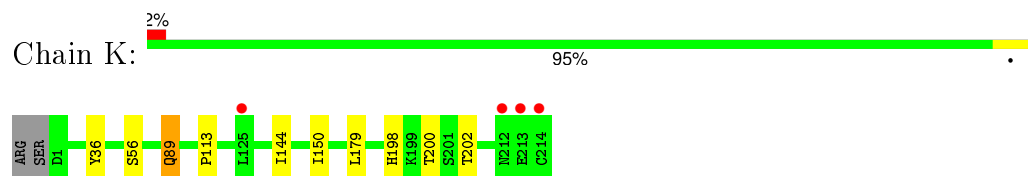
• Molecule 2: A13-D6.3 MONOCLONAL ANTIBODY



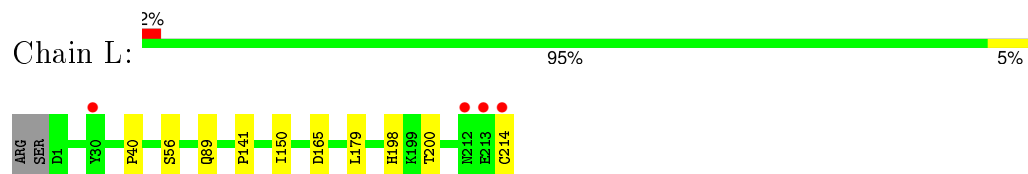
• Molecule 2: A13-D6.3 MONOCLONAL ANTIBODY



• Molecule 3: A13-D6.3 MONOCLONAL ANTIBODY



• Molecule 3: A13-D6.3 MONOCLONAL ANTIBODY



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.31Å 100.63Å 161.83Å 90.00° 94.02° 90.00°	Depositor
Resolution (Å)	58.12 – 2.05 55.64 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.8 (58.12-2.05) 92.1 (55.64-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.11.0	Depositor
R, R_{free}	0.188 , 0.205 0.190 , 0.208	Depositor DCC
R_{free} test set	7603 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 151525 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14739	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.05 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6582e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	1/3544 (0.0%)	0.63	0/4826
1	E	0.48	0/3544	0.64	1/4826 (0.0%)
2	G	0.49	0/1691	0.59	0/2309
2	J	0.54	0/1691	0.60	0/2309
3	K	0.52	0/1742	0.62	0/2367
3	L	0.53	0/1730	0.62	0/2353
All	All	0.50	1/13942 (0.0%)	0.62	1/18990 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	MET	SD-CE	-5.96	1.44	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	612	PRO	C-N-CA	5.61	135.72	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3475	0	3463	18	0
1	E	3475	0	3463	18	0
2	G	1648	0	1601	3	0
2	J	1648	0	1601	4	0
3	K	1698	0	1624	6	0
3	L	1689	0	1611	6	0
4	A	56	0	50	0	0
4	E	28	0	25	0	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
5	E	14	0	13	1	0
6	A	135	0	0	0	0
6	E	159	0	0	1	0
6	G	141	0	0	0	0
6	J	184	0	0	1	0
6	K	171	0	0	1	0
6	L	162	0	0	0	0
All	All	14739	0	13501	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 51 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:612:PRO:HB2	1:E:613:THR:HB	1.45	0.95
2:G:156:SER:H	2:G:196:ASN:HD21	1.30	0.77
1:A:337:GLN:HG2	3:L:56:SER:HB2	1.74	0.70
2:J:156:SER:H	2:J:196:ASN:HD21	1.40	0.69
3:L:150:ILE:HD11	3:L:179:LEU:HD21	1.81	0.61

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/572 (79%)	434 (96%)	17 (4%)	1 (0%)	52	43
1	E	452/572 (79%)	433 (96%)	15 (3%)	4 (1%)	21	10
2	G	212/261 (81%)	206 (97%)	6 (3%)	0	100	100
2	J	212/261 (81%)	207 (98%)	5 (2%)	0	100	100
3	K	217/220 (99%)	213 (98%)	4 (2%)	0	100	100
3	L	216/220 (98%)	209 (97%)	7 (3%)	0	100	100
All	All	1761/2106 (84%)	1702 (97%)	54 (3%)	5 (0%)	46	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	627	ASN
1	A	561	ALA
1	E	561	ALA
1	E	614	LEU
1	E	612	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/423 (82%)	333 (96%)	14 (4%)	38	29
1	E	347/423 (82%)	333 (96%)	14 (4%)	38	29
2	G	189/222 (85%)	187 (99%)	2 (1%)	80	79
2	J	189/222 (85%)	185 (98%)	4 (2%)	61	56
3	K	192/193 (100%)	190 (99%)	2 (1%)	82	81
3	L	191/193 (99%)	189 (99%)	2 (1%)	82	81
All	All	1455/1676 (87%)	1417 (97%)	38 (3%)	54	47

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	237	VAL
1	E	487	PRO
3	K	202	THR
1	E	432	LEU
1	E	559	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	557	GLN
1	E	611	ASN
3	K	198	HIS
1	E	542	ASN
3	K	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

10 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1101	1,4	14,14,15	1.35	2 (14%)	15,19,21	1.50	1 (6%)
4	NAG	A	1102	4	14,14,15	1.38	2 (14%)	15,19,21	1.09	2 (13%)
4	NAG	A	2101	1,4	14,14,15	1.52	1 (7%)	15,19,21	1.69	3 (20%)
4	NAG	A	2102	4	14,14,15	1.46	1 (7%)	15,19,21	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1101	1,4	14,14,15	1.28	3 (21%)	15,19,21	1.45	1 (6%)
4	NAG	E	1102	4	14,14,15	1.39	2 (14%)	15,19,21	0.96	1 (6%)
4	NAG	G	1101	2,4	14,14,15	1.93	2 (14%)	15,19,21	2.32	5 (33%)
4	NAG	G	1102	4	14,14,15	2.00	2 (14%)	15,19,21	1.82	3 (20%)
4	NAG	J	1101	2,4	14,14,15	1.90	3 (21%)	15,19,21	2.42	5 (33%)
4	NAG	J	1102	4	14,14,15	2.05	3 (21%)	15,19,21	1.80	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1101	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1102	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2101	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2102	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1101	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1102	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1101	2,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1102	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1101	2,4	-	0/6/23/26	0/1/1/1
4	NAG	J	1102	4	-	0/6/23/26	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	NAG	C3-C2	2.05	1.57	1.52
4	E	1101	NAG	C3-C2	2.07	1.57	1.52
4	J	1101	NAG	O4-C4	2.13	1.48	1.43
4	E	1101	NAG	C1-C2	2.17	1.55	1.52
4	E	1101	NAG	O5-C1	2.21	1.47	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1101	NAG	O4-C4-C3	-4.56	100.07	110.34
4	G	1101	NAG	O4-C4-C3	-4.53	100.13	110.34
4	J	1102	NAG	C3-C2-N2	-3.15	103.01	110.56
4	G	1102	NAG	C3-C2-N2	-2.78	103.91	110.56
4	A	1102	NAG	C6-C5-C4	2.03	118.03	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	E	2101	1	14,14,15	1.44	2 (14%)	15,19,21	0.91	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	2101	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2101	NAG	O5-C5	2.18	1.48	1.43
5	E	2101	NAG	C1-C2	2.41	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2101	NAG	C3-C2-N2	2.04	115.44	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2101	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	464/572 (81%)	0.70	57 (12%) 5 5	47, 73, 135, 168	0
1	E	464/572 (81%)	0.58	47 (10%) 9 10	45, 70, 124, 160	0
2	G	216/261 (82%)	0.49	7 (3%) 51 58	43, 61, 93, 130	1 (0%)
2	J	216/261 (82%)	0.50	5 (2%) 64 70	38, 53, 89, 141	1 (0%)
3	K	218/220 (99%)	0.28	4 (1%) 71 76	41, 58, 84, 123	0
3	L	218/220 (99%)	0.42	4 (1%) 71 76	40, 54, 87, 120	0
All	All	1796/2106 (85%)	0.53	124 (6%) 20 23	38, 63, 118, 168	2 (0%)

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	561	ALA	10.4
1	A	561	ALA	9.5
1	E	612	PRO	8.9
1	A	562	THR	8.7
1	A	560	PRO	7.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	E	1102	14/15	0.91	0.15	1.03	81,86,90,92	0
4	NAG	A	1102	14/15	0.94	0.12	0.14	77,82,85,88	0
4	NAG	E	1101	14/15	0.97	0.10	-0.40	72,77,81,81	0
4	NAG	A	1101	14/15	0.95	0.09	-0.96	66,71,75,75	0
4	NAG	J	1102	14/15	0.69	0.26	-	102,108,112,112	0
4	NAG	A	2102	14/15	0.78	0.45	-	179,183,189,192	0
4	NAG	G	1102	14/15	0.77	0.20	-	112,117,123,123	0
4	NAG	A	2101	14/15	0.76	0.40	-	169,172,179,183	0
4	NAG	J	1101	14/15	0.78	0.20	-	86,91,95,97	0
4	NAG	G	1101	14/15	0.86	0.18	-	98,104,108,108	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	E	2101	14/15	0.65	0.26	-	128,133,140,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.